

Electron-electron interaction effects in quantum point contacts

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(Dated: February 1, 2008)

We consider interaction effects in quantum point contacts on the first quantization plateau, taking into account all non momentum-conserving processes. We compute low-temperature linear and non-linear conductance, shot noise, and thermopower by perturbation theory, and show that they are consistent with experimental observations on the so-called "0.7 anomaly". The full temperature-dependent conductance is obtained from self-consistent second-order perturbation theory and approaches $\approx e^2/h$ at higher temperatures, but still smaller than the Fermi temperature.

PACS numbers: 72.10.-d, 73.23.-b, 72.10.Fk

Conductance quantization in a quantum point contact (QPC), first observed in 1988 [1], constitutes a classic textbook effect of mesoscopic physics. On top of the integer conductance plateaus $G = nG_0$ (where $G_0 = 2e^2/h$) observed as a function of gate voltage V_g , many experiments have pointed to the existence of a so-called "0.7 anomaly" in the conductance and other transport quantities [2, 3, 4, 5, 6]. Most prominently, the 0.7 anomaly implies a shoulder-like feature in the conductance $G(V_g)$ around $G \approx 0.7 G_0$ seen at elevated temperature T (or finite voltage V) near the first quantized plateau [2, 3, 4], accompanied by a shot noise reduction [6]. Given the conceptual simplicity of a QPC and the fact that the 0.7 anomaly has been observed in a variety of material systems by different groups over more than a decade, it is quite amazing that still no generally accepted microscopic theory exists, apart from an overall consensus that one is dealing with some spin-related many-body effect. Such a theory should be able to explain all the experimental data in a unified and physically consistent manner.

While phenomenological models [7], assuming the existence of a density-dependent spin gap, can provide rather good fits to experimental data, the presumed static spin polarization due to interactions within the *local* QPC region is not expected in the presence of unpolarized *bulk* reservoirs. Recently it was also pointed out that spin symmetry-broken mean-field theory is unable to recover the correct T dependence of the conductance [8]. Other proposals assume the existence of a quasi-bound state in the QPC region, leading to a Kondo-type scenario as encountered in transport through interacting quantum dots [9, 10]. Such a quasi-bound state was indeed found in spin density functional theory (SDFT) calculations [9], but other SDFT works did not reach such conclusions [11]. Further proposals involve phonon effects [12]. Several publications have suggested that taking into account only electron-electron (e-e) interactions may result in a reduced conductance at elevated temperatures, without the need for additional assumptions of spin polarization or a localized state [13, 14, 15, 16, 17]. However, a physically consistent picture explaining the temperature, voltage, and magnetic field dependence of the conductance,

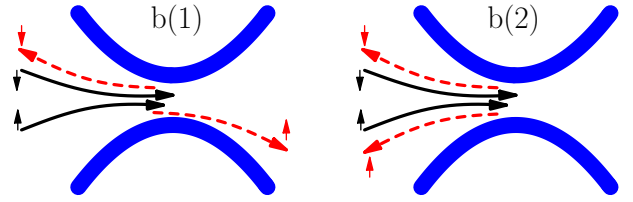


FIG. 1: (Color online) Illustration of the two-electron non momentum-conserving scattering processes that give rise to a correction to the transport properties at the beginning of the first plateau. The full (black) lines represent incoming electrons, while the dashed (red) lines are the outgoing electrons. The thick (blue) lines define the edge of the QPC. Only scattering between different spins is present to leading order in T/T_F due to the Pauli principle.

as well as thermopower and noise experiments, is still lacking. In this paper, we show that a careful consideration of *non momentum-conserving* e-e interaction processes in QPCs may allow for a consistent theory of the 0.7 anomaly.

The lack of momentum conservation in e-e scattering processes is due to an emerging lack of translational invariance relevant for the low density regime $k_F L \sim 1$, where k_F is the local Fermi momentum and L a typical interaction length-scale of the QPC (see below). Therefore this effect is dominant at the onset of the plateau and gradually disappears for larger electron density in the QPC. We will focus on the first conductance plateau, where the QPC has only one open channel (1D mode) [18, 19]. Now e-e interactions give the contribution

$$H_I = \frac{1}{2} \sum_{\sigma\sigma'} \int dx dx' W(x, x') \Psi_{\sigma}^{\dagger}(x) \Psi_{\sigma'}^{\dagger}(x') \Psi_{\sigma'}(x') \Psi_{\sigma}(x) \quad (1)$$

to the Hamiltonian, where $\Psi_{\sigma}(x)$ is the 1D electron field operator for spin $\sigma = \uparrow, \downarrow$. The pair potential $W(x, x')$ takes into account screening processes due to closed channels and nearby gates, as well as semiclassical slowing down [17], and therefore depends not only on the relative coordinate $x - x'$ but also on the center of mass $X = (x + x')/2$. In fact, the range of the interaction

$W(X)$ is determined by the above length-scale L . The e-e interaction now enters the 1D description in two different ways. There are (i) one-particle effects described through a self-consistent potential, given by the real part of the self energy (in the simplest case, this is the Hartree-Fock potential). At $T = 0$, the imaginary part of the self energy for our Fermi liquid starting point is zero [20], and the plateau then occurs where the open channel suffers no backscattering. This part is thus already contained in the potential forming the QPC. In addition, at finite T , we have (ii) inelastic e-e scattering processes, which are the focus of our work and give rise to a reduced conductance by changing the number of left- and right-movers, and hence the current. This is illustrated in Fig. 1, where two important types of non momentum-conserving scattering events are illustrated. Process b(2) describes the simultaneous backscattering of two electrons with opposite spins and has been discussed on a perturbative level in Ref. [14]. The process b(1), where a single electron is backscattered, has not been studied before. On top of these two, there are e-e forward scattering and backscattering processes (momentum-conserving in a long 1D wire). While high- T transport properties are affected by all interactions, we show now that the leading low- T behavior is *fully* determined by the two processes in Fig. 1.

Let us calculate the non-linear conductance, the thermopower, and the shot noise to leading order in the interaction. Perturbation theory gives the *interaction correction to the current* (here, $\hbar = 1$ and $e > 0$)

$$\frac{I(V, T)}{G_0 V} = 1 - (A_{b(1)} + A_{b(2)}) (\pi T / T_F)^2 - (A_{b(1)}/4 + A_{b(2)}) (eV / \varepsilon_F)^2 + \mathcal{O}(W^3), \quad (2)$$

with coefficients $A_{b(1,2)} = W_{b(1,2)}^2 k_F^4 / (48\pi^2 \varepsilon_F^2)$ corresponding to the b(1) and b(2) processes, where $\varepsilon_F = k_B T_F$ is the Fermi energy and $W_{b(1,2)} = \int dx dx' W(x, x') e^{ik_F(x+x')} e^{ik_F(x \mp x')}$. Already at this point, we observe a correspondence to experimental observations, namely the reduced conductance I/V with increasing T and/or V . Furthermore, to leading order in T/T_F , where all scattering happens at the Fermi level, only opposite spins interact due to the Pauli principle: for equal spins, the exchange term tends to cancel the direct term. As a consequence, we can also understand the behavior at *large magnetic fields*, where the $T = 0$ plateau occurs at e^2/h . In that case, to order $(T/T_F)^2$ no interaction renormalization of the conductance arises [21]. This is consistent with experiments, where no suppression is observed at the half-plateaus.

Another experimental observable probing the enhanced phase space for e-e scattering at higher T is the *thermopower* $\mathcal{S}(T)$ [22], for which perturbation theory predicts

$$\mathcal{S}(T) = \frac{k_B}{e} \frac{2\pi^4}{5} (A_{b(1)} + A_{b(2)}) (T/T_F)^3. \quad (3)$$

Since the non-interacting thermopower is exponentially small [$\propto \exp(-T_F/T)$] at the conductance plateau, the interaction correction completely determines the low-temperature thermopower [23]. The enhanced thermopower (as compared to the non-interacting one) is in qualitative agreement with experiments at the anomalous plateau [5].

Next we calculate consequences for another observable, namely non-equilibrium noise. The zero-frequency *shot noise* follows from the (symmetrized) two-point correlation function of the current operator. Perturbation theory yields for the backscattering noise power

$$S_B(V, T) = 2e \left[2I_{bs(2)}(V, T) \coth(eV/k_B T) + I_{bs(1)}(V, T) \coth(eV/2k_B T) \right], \quad (4)$$

where $I_{bs(1,2)}$ are the current corrections due to $W_{b(1,2)}$ quoted in Eq. (2) (defined positive for $V > 0$). This is nothing but the famous Schottky shot noise relation, encoding the charge of the backscattered particles. Equation (4) predicts an additional factor of two for the b(2) contribution, because two electrons are backscattered in that event [14]. Direct calculation then yields the full noise power of the transmitted current as $S_T = S_B + 4G_0 k_B T - 8k_B T \partial_V I_{bs}$, where $I_{bs} = I_{bs(1)} + I_{bs(2)}$. Recent noise measurements on the first quantized plateau were compared to the corresponding single-particle picture [6], and a reduced noise power was observed on the conductance anomaly. For that comparison, one subtracts the thermal noise and defines the excess noise as $S_I = S_T - 4G(V, T)k_B T$. For a non-interacting system, $S_I^{SP} = 2G_0 R \{eV \coth(eV/2k_B T) - 2k_B T\}$ to lowest order in the reflection coefficient $R = I_{bs}/G_0 V$, see Ref. [6]. Thus the difference between the true excess noise and its single-particle value is

$$\frac{S_I - S_I^{SP}}{2G_0 eV (T/T_F)^2} = -2A_{b(1)} \frac{eV}{k_B T} + A_{b(2)} h(eV/k_B T), \quad (5)$$

where $h(x) = -8x + (\pi^2 + x^2) \tanh(x/2)$. This expression shows that for $eV < 6.507 k_B T$, regardless of $A_{b(1,2)}$, the measured noise is always smaller than predicted by a single-particle analysis. This situation corresponds to the experimental work of Ref. [6], where $eV \lesssim 5k_B T$.

It is clear from all these perturbative results that for low energies, $V, T \rightarrow 0$, all interaction effects disappear. The perturbation theory results presented above, however, obviously break down at higher temperatures or voltages. From Eq. (2), we find the temperature scale for this crossover to a strong-interaction regime,

$$k_B T^* \approx \frac{\varepsilon_F}{\sqrt{A_b}} \propto \frac{\varepsilon_F^2}{W_b k_F^2}, \quad (6)$$

where $A_b = A_{b(1)} + A_{b(2)}$ and $W^2 = W_{b(1)}^2 + W_{b(2)}^2$. Contrary to the usual situation encountered in mesoscopic physics, the nontrivial question to be answered thus concerns the *high-temperature* limit (but still $T \ll T_F$). To

make progress in the relevant temperature regime

$$T^* \lesssim T \ll T_F, \quad (7)$$

let us consider a simplified model pair potential entering Eq. (1), see Ref. [17],

$$W(x, x') = V_0 \delta(x) \delta(x'), \quad (8)$$

which implies $W_{b(1)} = W_{b(2)}$. We express the interaction strength in the dimensionless parameter $\lambda = mV_0/2\pi^{3/2}$. Estimates for λ in GaAs heterostructures gives $\lambda \approx 1$, see Refs. [8, 17], which then yields $k_B T^*/T_F \approx 0.1$ allowing for a study of the temperature range (7).

In order to treat the local interaction (8), we start from the Dyson equation for the full Keldysh single-particle Green's function (GF) $\mathbf{G}(x, x'; \omega)$,

$$\mathbf{G}(x, x'; \omega) = \mathbf{G}_0(x, x'; \omega) + \mathbf{G}_0(x, 0; \omega) \mathbf{\Sigma}(\omega) \mathbf{G}(0, x'; \omega), \quad (9)$$

which is a 2×2 matrix in Keldysh space. The self energy due to Eq. (8) acts only at $x = x' = 0$. Note that $\mathbf{G}_\uparrow = \mathbf{G}_\downarrow$, i.e., we can suppress the spin index. For simplicity, we now assume a parabolic dispersion, $\varepsilon_k = k^2/2m$, for the open channel. The charge current operator is $I = \frac{ie}{2m} \sum_\sigma [\Psi_\sigma^\dagger(x) \partial_x \Psi_\sigma(x) - (\partial_x \Psi_\sigma^\dagger(x)) \Psi_\sigma(x)]$, and we evaluate $\langle I \rangle$ at $x = 0$, where it can be expressed in terms of the local GF $\mathbf{G}(\omega) \equiv \mathbf{G}(0, 0; \omega)$ and the self energy $\mathbf{\Sigma}(\omega)$. In fact, some algebra shows that only the local spectral function $A(\omega) = -2 \text{Im} G^r(\omega)$ enters the current formula for the contact interaction (8),

$$I = \frac{2e}{h} \int_0^\infty d\omega [f_R^0(\omega) - f_L^0(\omega)] \frac{A(\omega)}{A_0(\omega)}, \quad (10)$$

where $f_{R/L}^0$ are Fermi functions in the right/left lead, and $A_0(\omega) = 2\pi d(\omega)$ is the non-interacting spectral function. Here, $d(\omega)$ is the density of states $2\pi d(\omega) = (2m/\omega)^{1/2} \theta(\omega)$. Remarkably, the nonequilibrium current through the interacting QPC is thereby fully expressed in terms of the local retarded GF only. So far, the given relations are exact, but to make progress, one needs to approximate the self energy. We take the full *second-order self energy*,

$$\begin{aligned} \Sigma^r(\omega) = & V_0^2 \int_0^\infty dt e^{i\omega t} [G^<(-t)G^>(t)G^>(t) \\ & - G^>(-t)G^<(t)G^<(t)], \end{aligned} \quad (11)$$

and make it self-consistent by using the interacting (lesser/greater) GFs. The corresponding diagrams are shown in the inset to Fig. 2. The approximation (11) is the simplest way to describe equilibration between left- and right-moving electrons in an interacting QPC. In what follows, we confine ourselves to the linear conductance regime, where the spectral function in Eq. (10) can be calculated in equilibrium by solving Eq. (11), and where we can replace $f_R^0 - f_L^0 \rightarrow eV[-\partial_\omega f(\omega)]$, where $f(\omega)$ is the Fermi function. In linear response, the

lesser/greater GFs can be written in terms of the local spectral function $A(\omega)$,

$$G^{</>}(t) = \pm i \int_0^\infty \frac{d\omega}{2\pi} e^{-i\omega t} A(\omega) f(\pm\omega). \quad (12)$$

This suggests a natural iterative way to self-consistently solve for the conductance: Starting with the initial guess $A(\omega) = A_0(\omega)$, one computes $\Sigma^r(\omega)$ from Eq. (11), which in turn defines a new retarded GF and a new guess for $A(\omega)$. This procedure is iterated until convergence has been reached. For the parameters below, this numerical scheme is convergent and can be implemented in an efficient manner.

The numerical results, for $\lambda = 0.8$ shown in Fig. 2, accurately reproduce the above perturbative results at low T , but also allow to cover the interesting high-temperature limit. Our data for different λ fall to high accuracy on the simple function

$$\frac{G(T)}{G_0} = b + \frac{1-b}{1+(T/T_\lambda^b)^2}, \quad (13)$$

where b sets the high-temperature saturation value. While this functional dependence is somewhat similar to the phenomenological Kondo-type function used in Ref. [4], our numerical data fit better to Eq. (13). It is also possible to obtain equally good fits to the activated T dependence reported in Ref. [3], see also Ref. [7],

$$\frac{G(T)}{G_0} = 1 - (1-a)e^{-T_\lambda^a/T}, \quad (14)$$

where a again denotes the high- T limit. The values for T_λ^b and T_λ^a extracted from best fits to our numerical data are summarized in the inset in Fig. 2. Remarkably, both temperature scales are of the same order. Moreover, they are lowered by increasing the interaction strength λ . For high T , the conductance appears to approach the saturation value $G \approx e^2/h$. Similar saturation value has also been reported for *long* wires [13], with the same $T = 0$ conductance G_0 . The new feature for QPCs comes from the non-momentum conserving interactions, resulting in a distinct low-to-intermediate temperature dependence $G(T)$. The perturbative T^2 correction is not present in the long wire results [13], but is seen experimentally [4].

As a final remark on the numerical solution of the self-consistent approach, we mention that thermopower (data not shown) exhibits a crossover from the $\mathcal{S} \propto T^3$ law at low T , see Eq. (3), to a linear-in- T behavior at elevated temperatures.

It is also instructive to discuss our model in terms of an Anderson model. For the model pair potential (8), by spatial discretization our Hamiltonian maps to a 1D tight-binding chain with hopping matrix elements t and on-site interaction U acting at one site ($x = 0$) only [24]. We thus arrive at an Anderson-type impurity model, similar to the one used in Ref. [9] to describe interactions in a QPC in the Kondo regime. However, we consider a rather

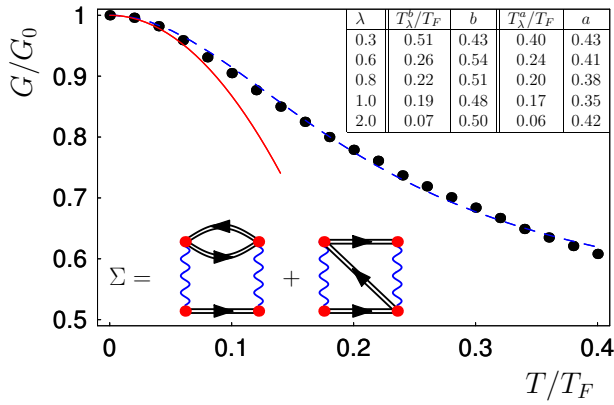


FIG. 2: (Color online) Temperature dependence of the linear conductance G for $\lambda = 0.8$. Dots denote self-consistent numerical results, the solid curve gives the perturbative estimate (2), and the dotted curve is a fit to Eq. (13). Inset: Fit parameters entering best fits of Eqs. (13) and (14) to numerical data for $T/T_F < 0.4$. Note that a and b are somewhat different. The lower inset shows the two second order self-consistent energy diagrams in Eq. (11).

different parameter regime, where U is of the same order as the hybridization Γ and can be parametrically larger than the bandwidth $D \sim |t|$. Employing Eq. (6), with $\varepsilon_F \approx D$, the interesting temperature range (7) translates to $D^2/U \ll k_B T \ll D$, where our claim is that G approaches $\approx e^2/h$. While the Kondo model requires the formation of a local moment, this is not the case for the

present approach. Instead, our high-temperature limit may be described as an *incoherent Fermi liquid*, with *full relaxation* between left- and right-movers. In fact, one can establish that a simple Boltzmann-type approach has a high-temperature solution where the out-going distribution function is a mixture of the incoming left- and right-mover's distributions. Such an Ansatz leads to the conductance formula (13) with $b = 1/2$, which is the reason for using that as a fitting formula. Unfortunately, a Boltzmann approach is conceptually difficult to justify due to an inherent normalization problem[17], i.e. one cannot define a proper local distribution function in k -space for this model.

In conclusion, we have considered interaction effects in short QPCs and shown that taking into account non momentum-conserving processes, we can qualitatively account for the experimentally observed behavior of the linear and non-linear conductance, thermopower (including their magnetic field dependencies) and shot noise at the so-called 0.7 anomaly. The gate voltage dependence can also be explained within the present scheme, because the backscattering is suppressed for larger values of $k_F L$. In the high-temperature (but still $T \ll T_F$) non-perturbative regime, our second-order self-consistent approach predicts that the conductance approaches $\approx e^2/h$. It is an open and interesting problem to verify this result by other non-perturbative methods.

We thank P. Brouwer, W. Häusler, and J. Paaske for discussions. This work was supported by the SFB TR 12 of the DFG and by the ESF network INSTANS.

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the one-particle on-site energy must be canceled out, so that $\epsilon_0 = -\text{Re}[\Sigma^r(0)]$ at zero temperature.